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Analysis of the Finite Mass Transfer Models in the Numerical Simulation of Bubbly Flows

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Abstract

In this study, the effect of empirical constants on the performance of the finite mass transfer models as well as some numerical issues of the model are investigated through the numerical analysis of the Rayleigh problem and the collapse of a bubble cluster. Also, by implementing the exact bubble radius profile into the model, it is shown that the pressure field can be very well estimated by the model.

Keywords: cavitation modeling; finite mass transfer model; bubble collapse

Introduction

A common numerical method for simulation of cavitating flows in large scale applications (e.g. marine propellers) is the homogeneous mixture modeling based on the finite mass transfer assumption. In this approach, the multiphase fluid is considered as a homogeneous mixture and a scalar transport equation is solved to find the liquid-vapor interface based on the interface-capturing scheme and the mass transfer between the phases is modeled using empirical terms. While these models are used to study turbulent sheet and cloud cavity structures with reasonable accuracy, they are limited in resolving small scale structures such as cavitation nuclei and bubbles. One source of such a limitation is the simplification behind the derivation of the mass transfer terms. In fact, most of the popular models are based on a simplified form of the well-known Rayleigh-Plesset equation in which the second-order derivative term is ignored. As cavity inertia becomes more important in the last steps of its collapse, such a simplification can decrease model accuracy in capturing bubble collapse and rebound. Further, some empirical coefficients are introduced to the mass transfer term which usually need to be tuned for different applications.

In this paper, the capability of the finite mass transfer model in the prediction of cavitating flows is investigated through a study of the effect of the empirical coefficients; also some numerical issues in pressure estimation are discussed. The Schnerr-Sauer model [1] is used to obtain mass transfer rate and two test cases are chosen for this study. The first case is the collapse of a vapor bubble under a far-field pressure higher than the characteristic vapor pressure. The second problem is the collapse of a cluster of bubbles in which the collapse of each bubble is influenced by the dynamics of surrounding structures. Then, a different approach is used to find the exact single bubble interface, which help to clarify one aspects of the mass transfer model limitation in appropriate estimation of pressure field of the cavitating flows.

Method

In this approach, the general continuity and Navier-Stokes equations are solved to calculate the main flow field and the interface capturing scheme based on the Volume of Fluid (VOF) concept is used to calculate the liquid-vapor interface. Therefore, a scalar transport equation for the liquid volume fraction, α, is solved and the liquid-vapor mass transfer at the interface is considered as a source term to this equation as

$$\frac{\partial \alpha}{\partial t} + \frac{\partial (u_i \alpha)}{\partial x_i} = \frac{\dot{m}}{\rho_l}, \tag{1}$$

where u_i is the velocity vector and ρ_l is the liquid density. There are various empirical models in literature to estimate the mass transfer rate, $\dot{m}$. In this study, the Schnerr-Sauer model [1] of OpenFOAM is used in which the condensation and vaporization rates are given by

$$\dot{m}_c = C_c \alpha (1-\alpha) \frac{3\rho_l \rho_v}{\rho_m R_B} \sqrt{\frac{2}{3\rho_l |p - p_{sat}|}} \max(p - p_{sat}, 0), \tag{2a}$$

$$\dot{m}_v = C_v \alpha (1 + \alpha_{Nuc} - \alpha) \frac{3\rho_l \rho_v}{\rho_m R_B} \sqrt{\frac{2}{3\rho_l |p - p_{sat}|}} \min(p - p_{sat}, 0). \tag{2b}$$

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where R_B and α_{Nuc} are the generic radius and volume fraction of bubble nuclei which can be considered as empirical parameters. ρ_v and ρ_m are the vapor and mixture density, respectively and p_{sat} is the saturation pressure of the fluid. Finally, C_c and C_v are the empirical condensation and vaporization coefficients implemented in OpenFOAM, respectively. R_B and ρ_m are functions of liquid volume fraction and are updated at each time step. To simplify the analysis, all other parameters are kept constant and only condensation and vaporization coefficients are modified. In this study, the liquid and vapor densities are 1000 kg/m^3 0.01389 kg/m^3, saturation pressure is 2330 kg/ms^2 and α_{Nuc} is set to 5*10^{-5} by considering 10^8 nuclei/m^3 with initial diameter of 0.1 mm.

The mixture properties (including density) are updated at each time step based on the liquid volume fraction at each cell. However, pure liquid and vapor are assumed to be incompressible. The governing equations are solved in the open source C++ package OpenFOAM using *interPhaseChangeFoam* solver.

Result

To investigate performance of the model, the simple problem of *Rayleigh bubble collapse* is studied first. For this problem, the analytical solution for evolution of bubble radius as well as its surrounding pressure are available in literature [2]. Here, the collapse of a vapor bubble in an infinite medium with atmospheric pressure is simulated and the effects of viscosity, non-condensable gas, and surface tension are ignored. The initial bubble radius is 0.4 mm and the vapor pressure is assumed to be 2340 Pa. Considering the spherical symmetry of the problem, only one cell layer of one eighth of the domain is simulated, using corresponding symmetry and wedge boundary conditions. The far-field is located 0.5 m from the bubble center. A polar grid is used to discretize the domain and the initial bubble is resolved with 20 radial cells (i.e. Δ_r/R_0 = 0.05, around the bubble). In figure 1, the generated grid and the initial Laplacian pressure field is depicted. The solution time step is 5*10^{-9} s.

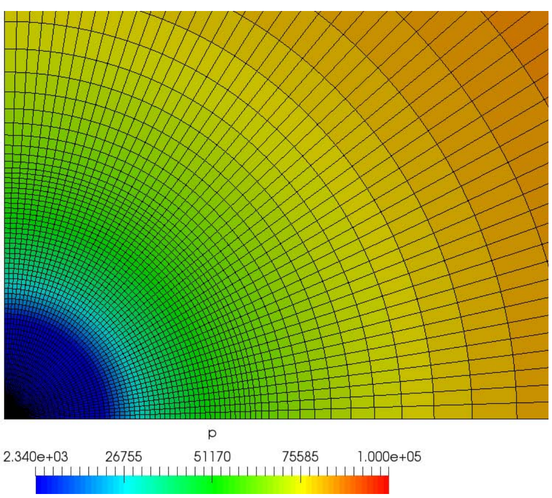

Figure 1: Domain discretization and initial pressure field

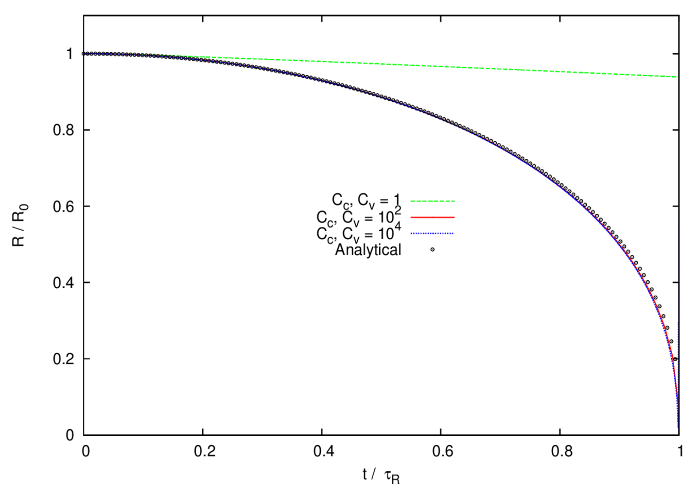

Figure 2: Temporal evolution of bubble radius

In figure 2, the temporal evolution of bubble radius with different mass transfer coefficients is compared with the analytical solution. The solution time and bubble radius are normalized with Rayleigh collapse time (τ_R) and initial radius (R_0), respectively. According to the figure, for small coefficients, the finite mass transfer model is incapable in estimation of bubble radius profile and the empirical constants should be larger than a minimum value. However, to have a better understanding of the model behavior, the calculated pressure profile should be investigated as well. In figure 3, the estimated pressure profiles in the radial direction around the bubble interface are compared to analytical data at three instances of the last stages of bubble collapse. In this figure the radial distance from the bubble center (R) is normalized with bubble initial radius (R_0) and the vertical axes shows the normalized pressure profile, given by $\Pi = (p - p_\infty)/(p_\infty - p_v)$. According to the figure, the pressure field is highly dependent on the mass transfer coefficients. In fact, while both moderate (C = 10^2) and large coefficients (C = 10^4) predict similar radius profiles, their pressure estimations are considerably different. For the lower coefficient, the estimated pressure inside the bubble is larger than the vapor pressure (Π > -1). Also, some numerical pressure pulses are emitted from bubble interface which makes the pressure values at t / τ_R = 0.921 to be larger than the corresponding values at a later time (t / τ_R = 0.948). If we increase the mass transfer coefficient to C = 10^4 these numerical pulses have almost disappeared from the solution and the pressure inside the bubble is estimated correctly. However, the pressure peaks around the interface is underestimated and the pressure lines are shifted a little as compared to analytical data. It can be shown that if the coefficients are increased further, the solution does not change. Therefore, to have an appropriate prediction of single bubble collapse, the coefficients should be set large enough. This conclusion is in agreement with results of Schenke and van Terwisga [3] using a different mass transfer model. It should be emphasized that increasing the model coefficients can cause numerical instability in the solution and special convergence measures should be applied to the solver to guarantee a converged and stable solution. To further investigate the model performance, the problem is solved with a coarser grid in which the initial bubble is discretized with 12 cells (i.e. $\Delta_r/R_0 = 0.083$). In figure 4, the calculated pressure profiles with empirical coefficients of 10^4 are compared with the corresponding ones of the fine grid. It is seen that, even with the high mass transfer coefficients, considerable numerical pressure pulses are existed in the solution when the grid resolution is not fine enough. This is an important point, since in typical engineering problems, the small cavity structures are not discretized with very fine grids.

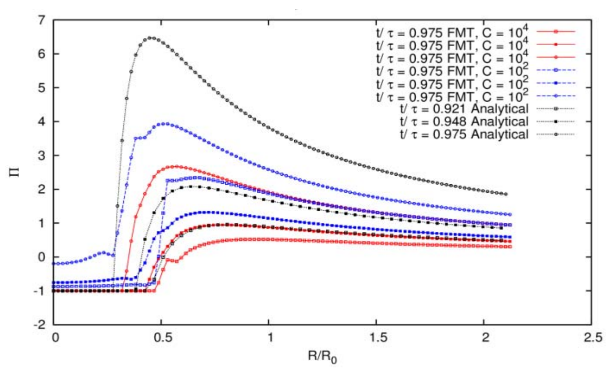

Figure 3: Pressure estimation of the finite mass transfer model with different empirical coefficients

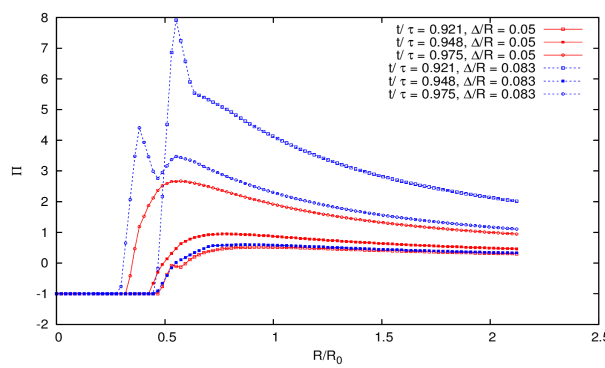

Figure 4: Pressure estimation of the finite mass transfer model with different domain discretization; $C = 10^4$

To study the mass transfer coefficient effect for more complex problems, the collapse of a cluster of bubbles is solved and the obtained solution is compared to the results of Schmidt et al. [4], where a compressible solver using thermodynamic equilibrium equation of state for the liquid, mixture, and vapor. In this problem, a cluster of 125 bubbles over a flat wall is exposed to an external pressure of 40 bar at infinity and the collapse resulting pressure impacts on a bottom wall are measured. The bubble cluster is in a small cube with an edge length of 20 mm. This cube is discretized uniformly by 55^3 cells. The farfield boundaries are located on the edges of a larger domain with $4*4*2$ m^3 dimensions and the solution time step is $3.9*10^{-8}$ sec. For further description of the problem, the reader is referred to [4]. Here, the collapse of each bubble can affect the pressure field around the surrounding bubbles. In figure 5 the obtained pressure impacts on the bottom wall are compared with the equilibrium model results for different mass transfer coefficients. From the equilibrium model result, it is seen that, due to the collapse of different bubbles, some pressure pulses are imposed on the wall which can be seen as local peaks in the plot. For the finite mass transfer model, however, the results are highly dependent on the mass transfer coefficient. If the coefficients are low, no pressure pulse is seen from individual bubble collapse and the wall pressure impact increases smoothly to the maximum value which corresponds to the final violent collapse and after the collapse it decreases smoothly. When the coefficients are increased to moderate values ($C = 10^2$), some pressure pulses are imposed on the wall and the maximum pressure value is estimated much larger than the corresponding value of compressible equilibrium model. When the coefficients are increased further to high values ($C = 10^4$), the peak pressure estimation is decreased again, and the local peaks of the profile are changed both in value and position. Also, according to the previous findings of single bubble collapse, it is not assured which of these local peaks are physical and which of them are only spurious numerical pulses.

To investigate possible sources of this inconsistency in the finite mass transfer approach, the simple Rayleigh collapse problem is considered again. For this problem, it is possible to have the exact bubble radius evolution from the solution of Rayleigh-Plesset equation. Then this exact profile of the cavity interface can be used investigate the model capability in prediction of collapse pressure. In other words, a modified finite mass transfer approach is used in which the exact volume fraction distribution is available from the Rayleigh-Plesset equation and the mass transfer model is only used to obtain the continuity equation source term to calculate the pressure field. The obtained pressure profile is compared to analytical data in figure 6, for both coarse and fine grids. In this case, the mass transfer coefficients are set to high values ($C = 10^4$). According to the fine grid solution, the pressure field can be very well estimated by the mass transfer model if the coefficients are high enough and the pressure peaks and their locations are well-captures without any shift in the profile. Also, from the coarse grid solution, it is concluded that, even with less accurate discretization, the model has an acceptable accuracy and no numerical pressure pulse is generated in the domain. It should be noticed that the previously mentioned numerical instability problems for the model do not exist in the new solutions. In summary, the mass transfer model can predict the pressure profile with reasonable accuracy and without any numerical issue, provided that the coefficients are high enough. In other words, one major source of the mass transfer model inconsistencies in prediction of cavitation problems is in the solution of the scalar transport equation of the liquid volume fraction. Inheriting the interface capturing scheme nature, this equation needs very fine grid and special solution criterion to sufficiently resolve the cavity interface and avoiding numerical pulses. Also, in order to have more stable solution and diagonal dominancy of the coefficient matrix this equation is usually discretized as

$$\frac{\partial \alpha}{\partial t} + \frac{\partial (u_i \alpha)}{\partial x_i} = \frac{\dot{m}}{\rho_l} + \alpha \left(\frac{\partial u_i}{\partial x_i} - \frac{\partial u_i}{\partial x_i} \right). \tag{4}$$

While theoretically, the two velocity divergence terms should be identical, one term is replaced by the continuity equation source term and the other term is calculated from the velocity field. Since the continuity equation and the volume fraction transport equations (and its corresponding source term) are not solved simultaneously for each solution iteration, these two terms are not necessarily equal and it can cause some numerical error in the solution of the volume fraction transport equation.

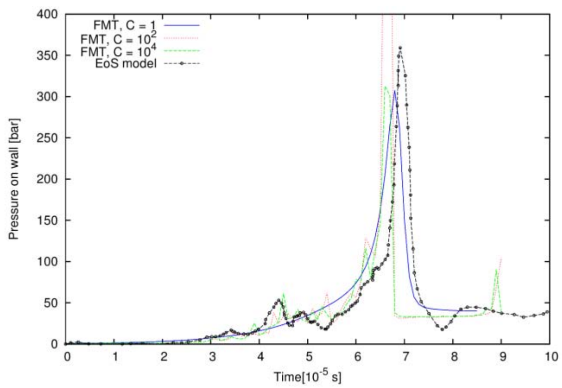

Figure 5: Pressure impact estimation of the finite mass transfer model with different coefficients for the collapse of a bubble cluster

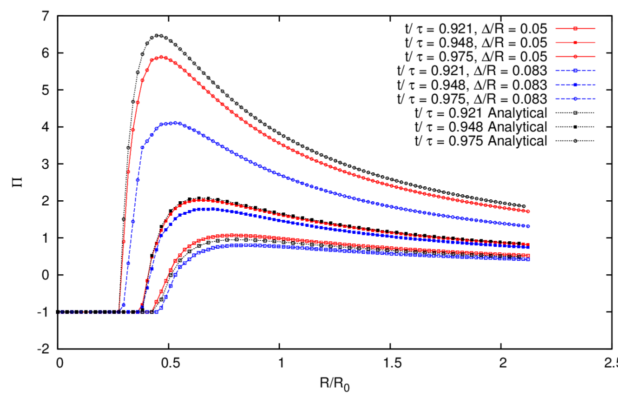

Figure 6: Estimated pressure profile of the finite mass transfer model with the exact solution of the bubble interface

Conclusion

From the solution of the single bubble collapse, it is concluded that for resolving the collapse event the empirical coefficients of the mass transfer model should be large enough and very fine grids are needed. Otherwise, the bubble collapse may have numerical delay for small coefficients or numerical pulses may happen. This can be problematic for the more complex cases when the collapse of each bubble may influence the dynamics of other structures. It is shown that a major source of this issue is the numerical problems in solving of vapor transport equation.

Acknowledgement

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